

# The State of $\text{Be}^7$ in the Core of the Sun and the Solar Neutrino Flux

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## ABSTRACT

The exact ionization state of  $\text{Be}^7$  in the solar core is crucial for the precise prediction of the solar  $\text{B}^8$  neutrino flux. We therefore examine the effect of pressure ionization on the ionization state of  $\text{Be}^7$  and all elements with  $12 \geq Z \geq 4$ . We show that under the conditions prevailing in the solar core, one has to consider the effect of the nearest neighbor on the electronic structure of a given ion. To this goal, we first solve the Schrödinger and then the Kohn-Sham equations for an ion immersed in a dense plasma under conditions for which the mean interparticle distance is smaller than the Debye radius. The question of which boundary conditions should be imposed on the wave function is discussed, examined and found to be crucial.

Contrary to previous estimates showing that Beryllium is partially ionized, we find that it is fully ionized. As a consequence, the predicted rate of the  $\text{Be}^7 + e^-$  reaction is reduced by 20-30%, depending on the exact solar model. Since  $\text{Be}^7$  is a trace element, its total production is controlled by the unchanged  $\text{He}^4 + \text{He}^3$  reaction rate, and its destruction is determined by the rate of electron capture. As the latter rate decreases when the Beryllium is fully ionized (relative to the case of partially ionized Be), the estimate for the abundance of  $\text{Be}^7$  increases and with it the  $\text{B}^8$  neutrino flux. The increase in  $\phi_\nu(\text{B}^8)$  is by about 20 – 30%. The neutrino flux due to  $\text{Be}^7$  electron capture remains effectively unchanged because the change in the rate is compensated for by a change in the abundance. Hence the prediction for the ratio of  $\phi_\nu(\text{B}^8)/\phi_\nu(\text{Be}^7)$  changes as well.

**Key words:** Sun:interior, equation of state, atomic processes, plasmas

## 1 INTRODUCTION

Classical calculations of solar models assume that all species are fully ionized above  $\sim 10^6\text{K}$  (e.g. ?). The main reason probably being the saving of computer time, because detailed ionization calculations are very CPU demanding. Alternatively, one can use tables for the equations of state which are calculated to high accuracy. However, one then has to interpolate for the relative abundances which change continuously once diffusion takes place. Indeed, from the point of view of the total gas pressure and other thermodynamic quantities, the partial (or complete) ionization of heavy species like C, N, O, Mg or even Fe, affect the number of free electrons at temperatures above a few million degrees at a relative level of about  $10^{-3}$ , depending on the exact mass fraction of the heavy elements. Consequently, the total pressure and speed of sound are affected at the same relative level of accuracy.

Iben Kalata & Schwartz (?, hereafter IKS67) examined the ionization state of  $\text{Be}^7$  in the solar core, and concluded that its K-shell electrons are partially bound (with a population level of about 30% depending on the exact location in the core). This fact significantly affects the predicted  $\text{B}^8$  neutrino flux from the Sun. The most important channel for the destruction of  $\text{Be}^7$  in the Sun is via electron capture, of which most are free electrons. However, if the  $\text{Be}^7$  ion has some bound electrons then the rate of electron capture is enhanced, and with it the generated  $\text{Be}^7$  electron capture neutrino flux (by about 20-30% once averaged over the entire relevant region in the Sun). Thus, the exact occupation fraction of the  $\text{Be}^7$  K-shell is important for the accurate prediction of the solar neutrino flux, and the ratio  $\phi_\nu(\text{B}^8)/\phi_\nu(\text{Be}^7)$  in particular. To include the effects of the plasma, IKS67 assumed a Debye Hückel (DH) potential and calculated the dependence of the ground state energy on the environmental conditions.

The problem of obtaining the ionization state of Beryllium in the Sun was later revisited by ?). The authors analyzed the validity of the Debye-Hückel potential and found that the prerequisites for the validity are weakly violated. The authors claim that once the assumptions for the validity of the DH are strongly violated, “experiments show that the DH fails dramatically”. In particular, we note the first point raised by the authors, namely the requirement to have many particles in a Debye sphere needed for the validity of the DH treatment. This requirement implies that the interparticle distance is significantly smaller than the Debye radius. The authors solve for the Beryllium atom assuming a DH potential using three different methods (DH, self-consistent DH and Hartree) and find only small differences in the ionization compared to IKS67.

?) discussed the ionization state of Beryllium in the Sun assuming mean field screening, the density matrix formulation, and a Monte Carlo method. However, all within the framework of a screened Coulomb potential. The authors also discussed the effects of fluctuations and found only minor effects.

If indeed Beryllium is partially ionized in the solar core, namely, it keeps the K-shell electrons at least part of the time, then several additional consequences follow. These effects were hitherto neglected in the prediction of the solar neutrino fluxes (predictions that assumed at the same time partial ionization of  $\text{Be}^7$ ).

First, the screening of the nuclear reaction  $\text{Be}^7 + p$ , which is the competing  $\text{Be}^7$  destruction reaction, should be calculated using the proper effective charge of the Be ion. Currently it is assumed to always have a charge of  $+4e$ . This effect would decrease the  $\text{B}^8$  neutrino flux.

Second, a similar correction to the screening should apply to the higher Z reactions of CNO+p, affecting in this way the (small) contribution of the CNO cycle to the total solar energy budget. This effect would suppress the CNO energy production because the effective charge of the ion would be smaller and hence the electrostatic screening energy would be smaller as well.

Third, the exact point at which various ions become completely ionized affects the entropy density in the outer convective zone of the sun, and with it the solar structure.

As the accurate prediction of the solar neutrino flux is so important, the purpose of this contribution is to re-examine the ionization state of the heavy species in the solar core, and in particular the ionization state of the trace element  $\text{Be}^7$ .

The question to which extent does the  $\text{Be}^7$  or any other heavy ion, retain its K-shell electrons is usually analyzed in two steps (IKS67). The first step is to apply the simple Saha equation assuming that the structure of the  $\text{Be}^7$  atomic energy levels is unaffected by the dense plasma. The second step is to account for the effect of the plasma on the energy levels of the  $\text{Be}^7$  by assuming a smooth DH potential and calculating the energy levels under the DH potential. Once the new energy levels are known, the electron population in the levels can be re-evaluated using a Saha equation which incorporates the revised energy levels. This approach is justified only as long as the plasma effects are small perturbations.

As we shall show, the conditions in the core of the Sun are very peculiar and the number of particles inside a Debye

sphere,  $N_D \approx \text{few}$  and *not* very large compared to unity. Hence, the necessary condition for the validity of the Debye Hückel theory is not satisfied. Moreover, the conditions in the core of the Sun are such that the mean distance between ions in general,  $\langle r_s \rangle = (4\pi n/3)^{-1/3}$ , and between a proton or an  $\alpha$ -particle and a Beryllium ion in particular, is of the order of  $2R_B(Z=4)$  (the Bohr radius in a nucleus with charge  $Z=4$ ) and hence the picture of an ion with an electronic shell inside a Debye-Hückel potential, is not strictly valid. Here,  $n$  is the number density of ions while the index  $s$  in  $\langle r_s \rangle$  corresponds to a calculation employing spherical packing of ions. When the DH theory applies, it means that there are many ions inside a Debye radius and the mean distance between ions is much smaller than the Debye radius. The electronic structure of the ions is then affected first and foremost by the close ion rather than by the Debye cloud and its large radius. This point, which is essential in this paper, will be discussed at length since this situation dictates a different boundary condition which subsequently leads to different energy levels and a different ionization state (under the same thermodynamic conditions).

The paper is structured as follows. We first question and analyze the effective potential to be used under the conditions prevailing in the solar core. Then we repeat the two steps analysis of IKS67. We next proceed to examine the pressure ionization at  $T=0$  assuming a Coulomb potential. In view of the doubtful validity of the DH potential under the conditions prevailing in the core of the Sun, we repeat the calculation assuming the Schrödinger and later the Kohn-Sham equations. We find that  $\text{Be}^7$  is fully ionized at a lower density (and temperature) than previously calculated. Finally, we examine the effect of the complete ionization of  $\text{Be}^7$  on the predicted solar neutrino flux according to different sets of nuclear reaction cross sections.

## 2 WHICH POTENTIAL?

The classical calculation of the atomic energy levels and pressure ionization assumes a smooth (in time and space) potential. We first examine the assumption that any applied potential can be assumed to be smooth for the specific problem of the structure of the electronic level of a given ion under the conditions prevailing in the core of the Sun.

For the assumption that the potential is smooth to be valid, the fluctuations of the plasma must be much faster than the motion of the electron in the bound orbit such that the average smooth value can be taken (for the calculation of the bound state) rather than the instantaneous one. We assume at the beginning that the plasma does not affect the energies of the bound levels. (The effect of the plasma is to make the energy levels shallower so the electrons would move even slower. Thus, the argument presented here is a conservative one.)

The Bohr radius in a Hydrogen-like ion with a charge  $Z$  (in vacuum) is given by:

$$a_0 = \frac{\hbar^2}{4\pi^2 m_e e^2 Z} = \frac{1}{Z} 0.528 \times 10^{-8} \text{cm}. \quad (1)$$

The classical velocity is:

$$v = 2Ze^2 \left( \frac{\pi}{\hbar} \right)^{1/2}, \quad (2)$$

and the period is

$$P = \frac{h^3}{4\pi^2 m_e e^4 Z}. \quad (3)$$

There are two sources for fluctuations in the potential, those caused by the protons and those caused by the electrons. The typical time scales of the fluctuations are

$$\tau_e = \frac{\langle r_s \rangle}{v_{th} (ZN_D)^{1/2}} = \frac{\langle r_s \rangle m_e^{1/2}}{(3kT)^{1/2} (ZN_D)^{1/2}} \quad (4)$$

$$\tau_p = \frac{\langle r_s \rangle}{v_{th} N_D^{1/2}} = \frac{\langle r_s \rangle m_p^{1/2}}{(3kT)^{1/2} N_D^{1/2}}, \quad (5)$$

where  $\langle r_s \rangle = 1/(4\pi n_{\text{ion}}/3)^{1/3}$  is the mean interparticle distance and  $n_{\text{ion}}$  is the number density of ions.  $v_{th}$  is the relevant thermal velocity. The number of particles in the Debye sphere is given by:

$$N_D = \frac{4\pi}{3} R_D^3, \quad (6)$$

where

$$R_D = \sqrt{\frac{kT}{4\pi e^2 \sum_j (Z_j^2 + Z_j) n_j}} \quad (7)$$

is the Debye radius for this mixture.  $n_j$  is the number density of specie  $j$  with charge  $Z_j$ . The above expression for the Debye radius assumes that both the electrons and ions contribute to the supposedly DH potential. For simplicity we assume  $N_D^{1/2} \approx 3$  and obtain that for  $n = 10^{26} \text{ #/cm}^3$ ,  $T = 1.5 \times 10^7 \text{ K}$  and a pure Hydrogen plasma,

$$\frac{P}{\tau_e} \approx 0.5 \quad \text{and} \quad \frac{P}{\tau_p} \approx 0.01. \quad (8)$$

Note that when some of the ions are Helium ions (in the core of the present Sun about half the ions are He),  $N_D$  decreases even more. What is the implication of this result? The fluctuations due to the electrons are of about the same timescale as the period of the electrons in the K-shell in a single ion in vacuum, while the protons in the plasma have a much longer time scale. Hence, it is not justified to treat the contribution of the electrons to the DH potential (felt by the electron) as a smooth potential in time. On the other hand, since there are only few protons in the Debye radius their contribution to the potential is smooth in time but not in space and certainly not spherical. Additional arguments that question the validity of the potential are given by ?). In what follows, we assume that all potentials are temporally smooth and spatially spherical.

### 3 THE IONIZATION OF BERYLLIUM IN THE SUN

#### 3.1 The state of ionization ignoring plasma effects

Next, we discuss the ionization state of  $\text{Be}^7$  in the core of the Sun - the classical way. If one adopts the Saha equation, ignoring screening and the excited energy levels (thus including only the ground states in the partition functions), then the probabilities  $f_1$  and  $f_2$  that one or two K-shell electrons are associated with any given  $\text{Be}^7$  nucleus are given by

(IKS67)

$$\begin{aligned} f_1 &= \frac{\eta}{1 + \eta + 0.25\eta^2 \exp(-\delta\chi/kT)}, \\ f_2 &= 0.25\eta \exp(-\delta\chi/kT) f_1, \end{aligned} \quad (9)$$

where

$$\eta = n_e \left( \frac{h^2}{2\pi m k T} \right)^{3/2} \exp(\chi_1/kT). \quad (10)$$

Here  $\chi_1 = 216.6 \text{ eV}$  is the forth ionization potential of the  $\text{Be}^7$  atom,  $\chi_2 = 153.1 \text{ eV}$  is the third ionization potential of the  $\text{Be}^7$  atom, and  $\Delta\chi = \chi_1 - \chi_2 = 63.5 \text{ eV}$ . These values correspond to the limit of vanishing plasma density.  $n_e$  is the number density of the free electrons, most of which are contributed by Hydrogen and Helium and are independent of the state of trace elements like Beryllium. Thus,  $n_e$  can be treated as fixed.

The application of the Saha equation in the above form to the core of the Sun ( $\rho = 158 \text{ g cm}^{-3}$ ,  $T = 1.57 \times 10^7 \text{ K}$ ,  $X = 0.36$  &  $Z = 0.02$ ) yields  $f_1 = 0.320$  and  $f_2 = 0.038$ , implying that the  $\text{Be}^7$  keeps its last electron for about a third of the time.

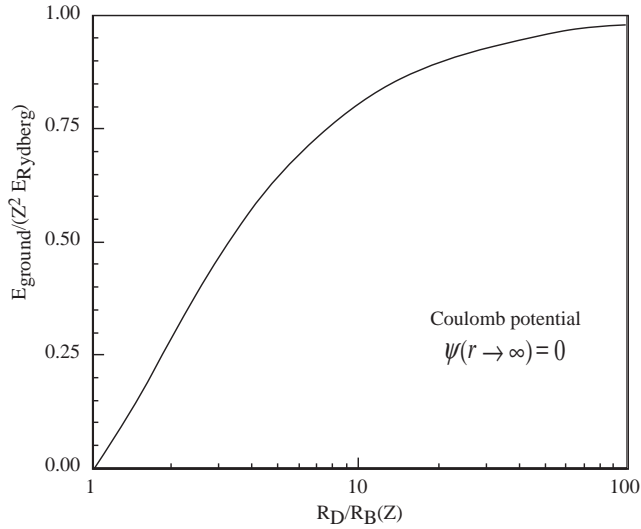
As the relevant ions are in a plasma, the traditional procedure to correct for the plasma effect is to replace the pure Coulomb potential with a DH one (?). This is for example the procedure IKS67 evaluated the plasma corrections for the energy levels of  $\text{Be}^7$  in the solar core.

The Saha equation in the above form ignores electron degeneracy, exchange effects and pressure ionization. The electron degeneracy introduces a small correction under the conditions prevailing in the Sun. As we will shortly demonstrate, exchange and pressure ionization are significantly more important. In what follows we do assume in spite of the previous reservations, a smooth static DH potential contributed by the electrons and ions. Moreover, we assume it to be relevant in a statistical sense only.

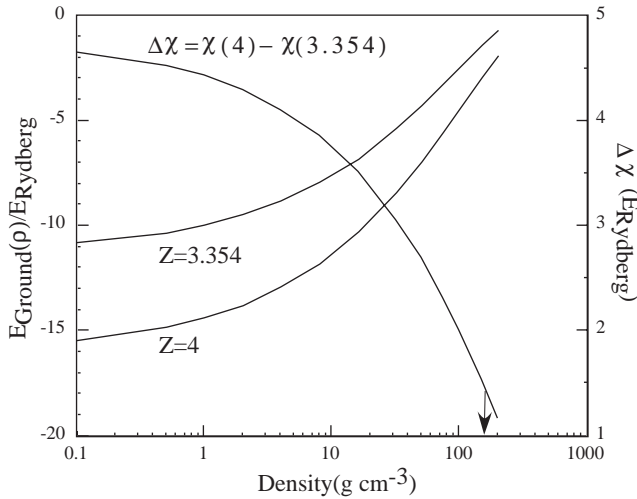
#### 3.2 Screened potential: taking into account the plasma effects

After performing the above estimate, IKS67 turned to evaluate the ground state of the  $Z = 4$  ion assuming a smooth DH screened potential in which both the protons and the electrons are taken into account. We ignored the questions raised in the previous section concerning the validity of the potential for our particular purpose here (ionization in the core of the Sun), repeated their calculation and confirmed their results with respect to the Hydrogen like ion with  $Z = 4$ . ?) calculated the bound states of static screened coulomb potential and formulated their results in terms of the screening length. We also repeated their results for the  $1s$  state and the results are shown in fig. 1. Clearly, as the Debye length approaches the Bohr radius of ions with charge  $Z$ , there are no more bound states. The boundary condition on the wave function in this case is  $\psi(r \rightarrow \infty) = 0$ .

The calculation of the plasma effects on the triply ionized  $\text{Be}^7$  ion is more complicated because of the partial screening of the nucleus by the bound electron. To overcome this problem, we used the following approximate method. We looked for the eigenvalue in the low density limit and searched for the effective charge that will reproduce the measured ionization potential of  $153.1 \text{ eV}$ . We found that this

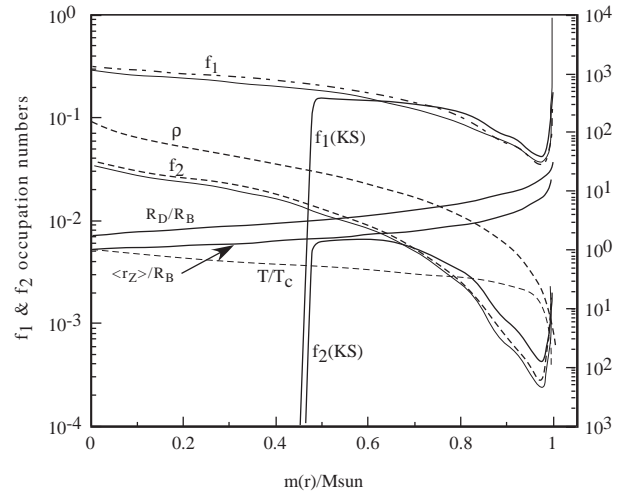


**Figure 1.** The energy of the ground state for a screened Coulomb potential as a function of the screening length. Note the units of the energy ( $Z^2 E_{\text{Rydberg}}$ ) and Debye length scale ( $R_D/R_B(Z)$ ) where  $R_B(Z)$  is the Bohr radius of an ion with charge  $Z$ .

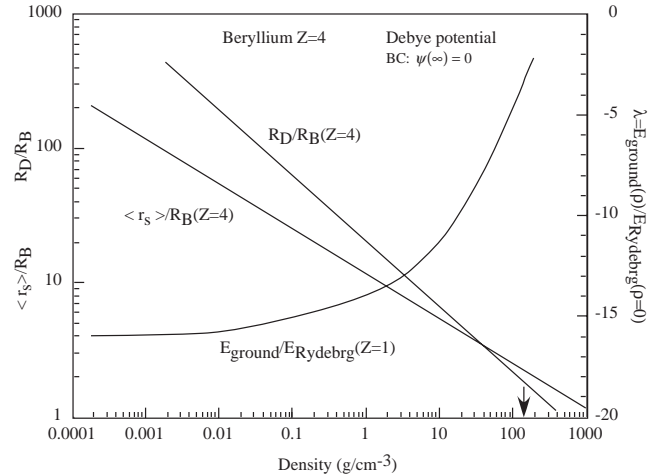


**Figure 2.** The run of the ground energy levels of a Be ion with one and two electrons as a function of density for a Debye Hückel potential and  $\psi(r \rightarrow \infty) = 0$  as the boundary condition. The temperature, which enters via the Debye radius, is taken as constant at  $1.57 \times 10^7 \text{ K}$ . Note that the temperature in the Sun decreases with density and hence the temperature and with it the Debye radius are overestimated here for densities lower than  $150 \text{ g cm}^{-3}$ . The correction for the accurate temperature is small. The purpose of the figure is to show the conditions in the solar core. The small arrow marks the density at the core.

charge is  $Z = 3.3544$ . We then repeated the calculation of the plasma effect on the bound states assuming this charge. The results are shown in fig. 2. We then used the new values for the ionization potential in the Saha equation to find the revised  $f_1$  &  $f_2$ . The comparison between the values used with and without the plasma correction is shown in fig. 3, where the actual run of the occupation numbers in the Sun is given. It is surprising that the differences in the ionization come out to be quite small.



**Figure 3.** The occupation numbers  $f_1$  and  $f_2$  of Be throughout the Sun as a function of the solar mass fraction. The broken lines are the results of IKS67. The continuous lines are the present results after incorporating the effective charge of the  $\text{Be}^{3+}$  ion ( $Z_{\text{eff}} = 3.354$ ). The curves marked with  $f_1(KS)$  and  $f_2(KS)$  are the results assuming  $\psi' = 0$  on the cell boundary. These results are the actual run of the occupation numbers in the Sun. Also shown are the density and temperature (in units of the central temperature) in the present day Sun. The run of  $R_D/R_B$  and  $\langle r_Z \rangle / R_B$  are shown as well.  $T/T_c$ ,  $\rho$ ,  $R_D/R_B$  and  $\langle r_Z \rangle / R_B$  are all shown on the left axis. The occupation numbers are shown on the right axis.



**Figure 4.** The run of the energy of the ground state as a function of density assuming fixed temperature and composition. Also shown are  $R_D/R_B(Z = 4)$  and  $\langle r_s \rangle / R_B(Z = 4)$ . The arrow marks the density in the center of the Sun.

The particular results for the binding energy (calculated for a DH potential) as a function of the density are shown again in figure 4 along with the run of the ratios  $R_D/R_B(Z = 4)$  and  $\langle r_s \rangle / R_B(Z = 4)$ . The Debye radius and the mean interparticle distance are calculated assuming  $X = 0.34$ ,  $Y = 0.68$  and  $Z = 0.02$ , a composition which is close to the one at the solar core today.

We notice that when the density approaches the density in the solar core, namely about  $150 \text{ g cm}^{-3}$ , (a) the Debye radius becomes of the order of the mean interparticle

distance and hence the approximation of a smooth Debye screened potential loses its validity, emphasizing once more the conclusion reached in section 2. (b) In the solar core, we find that  $R_D \approx R_B(Z = 4)$  and therefore the probability for complete ionization of the Be is very high.

However, the more important question here is the ratio of the mean interparticle distance to the Bohr radius since we are interested in the possibility that the ions of Beryllium still have bound electrons. Fig. 4, which depicts a graph for the value of  $\langle r_s \rangle$ , indicates that this value at the center of the Sun is close to  $R_B(Z = 4)$ . Therefore, it is a delicate question whether the Beryllium ions possess any bound electrons. Finally, we point out that  $\langle r_s \rangle$ , which is depicted in the figure, is the mean interparticle distance irrespective of their type. As we shall show, it is an underestimate in the case of a Beryllium ion embedded in Hydrogen and Helium ions.

## 4 PRESSURE IONIZATION AT $T = 0$

### 4.1 The boundary conditions

As discussed above, the classical method to evaluate the degree of ionization in a stellar plasma with a finite temperature is first to assume given mean distances between the particles, and assume that they are at rest, namely that  $T = 0$ . (However, we do keep the finite temperature in the calculation of the Debye radius). Once the energy levels are known, the effect of the temperature via the Boltzmann relation (leading to the Saha equation) is taken into account. In an actual plasma, the distance between the particles has a distribution and hence there is a distribution of cases. One assumes that the average of the results for the distribution is equal to the result for the average. We turn now to the  $T = 0$  case.

The question of pressure ionization is discussed by ?) within a general discussion about the energy levels of atoms in plasma and follows ?) and ?), where the effect of the plasma was simulated by a screened potential. Pressure ionization depends primarily on the density. However, when the relevant scale is the Debye length, some effect of the temperature on the energy levels enters through the back door via the dependence of the Debye screening length on the temperature, which as stated before we do keep finite in the calculation of the potential (in the case that a DH potential is assumed).

We distinguish between two possible situations:

Case A:  $R_D \gtrsim \langle r_s \rangle$  or  $N_D \gtrsim 1$  and

Case B:  $R_D \lesssim \langle r_s \rangle$  or  $N_D \lesssim 1$ .

The physical difference between the two cases is expressed in the boundary conditions imposed on the wave function in the problem of the electronic structure of the ion. In the first case, the nearest neighbor is closer than the Debye distance and hence one expects it to affect the electronic structure of the ion much more than the fact that the two ions are inside the same potential well. In the second case, the nearest neighbor is further away than the Debye radius and hence the boundary condition on the wave function with a DH potential can be  $\psi(r \rightarrow \infty) = 0$ . On the other hand, in the first case, the boundary condition should take into account the close ion. As the speed of the perturbing ions is of the same order as the speed of the ion under

consideration, the effect of the ions inside the Debye sphere cannot be averaged into a mean potential. The basic requirement to consider the effect of the nearest neighbor directly (and not via a smooth potential averaged over many ions) leads to the idea of a Wigner-Seitz unit cell or ion-sphere.

We can look also on the problem in the following way: If the bound state electronic wave function of a given ion overlaps significantly the bound electronic wave function of nearby ions the electron cannot be considered as bound (cf. ?).

We approached the problem of pressure ionization at  $T = 0$  in two steps which represent successive approximations. In the first step we solve the Schrödinger equation for the  $\text{Be}^7$  ion under the assumption that there is another nucleus at a distance  $\langle r_s \rangle$  away. In our particular case, the plasma contains ions with different charges and one cannot state that the ion sphere of all ions is identical. Hence the boundary condition must be imposed at  $\langle r_z \rangle = \alpha \langle r_s \rangle$ , where  $\alpha$  is soon to be determined. In the pure periodic case one should apply the Bloch condition (?, see also ?). We assume for simplicity spherical symmetry and hence the Bloch condition becomes the requirement that

$$\left. \frac{d\psi}{dr} \right|_{r=\alpha \langle r_s \rangle} = 0. \quad (11)$$

The coefficient  $\alpha$  is determined from the condition that the force vanishes at this point. Consequently, all wave functions we experimented with contained the condition that  $\psi'$  vanishes at  $\langle r_z \rangle = \alpha \langle r_s \rangle$ , namely contained the factor  $(r - \alpha \langle r_s \rangle)^2$ . Here  $\langle r_s \rangle$  is the distance to the nearest ion irrespective of its charge (in spherical packing). Note that in the Sun  $\text{Be}^7$  is a trace element and hence the nearest neighbor would most probably be a proton or a Helium nucleus. The approximation can be considered as a muffin-tin potential with a modified cell size, namely Coulomb inside  $\langle r_z \rangle$  and constant outside (cf. ?). It is obvious that imposing the above condition on the trial function increases the eigenvalue and hence ionization would occur, assuming all other conditions are unchanged, at a lower density.

Since we have a mixture of various ions, the point at which the force between ions vanishes varies with the ion. If our ion has a charge  $Z$ , then the corresponding ionic radius  $\langle r_z \rangle$  is given by:

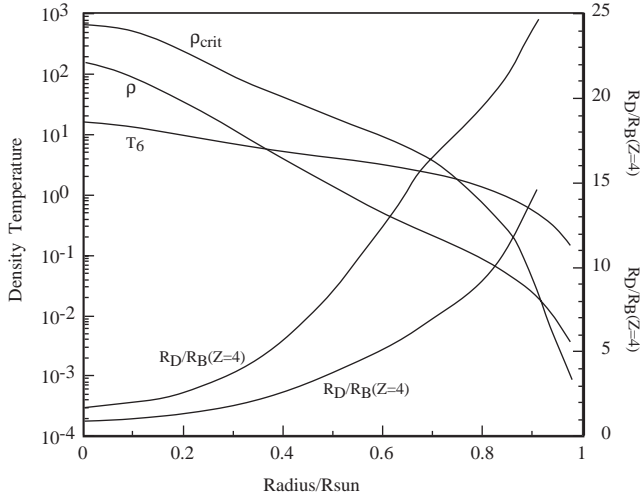
$$\langle r_z \rangle = \frac{\delta}{1 + \delta} \langle r_s \rangle \quad \text{where} \quad \delta = \left( \frac{Z \sum X_i Z_i / A_i}{\sum X_i / A_i} \right)^{1/2}. \quad (12)$$

If all ions are equal, then  $\langle r_z \rangle = (1/2) \langle r_s \rangle$ . Clearly, the above definition is a generalization of the Wigner-Seitz cell idea to a mixture of species. In the present case, we assume the electron to be localized in the Wigner-Seitz cell. We will define complete ionization when the localization of the electron ceases. In the DH case, there is no such assumption. Nevertheless, there are other ions (and electrons) moving inside the Bohr radius.

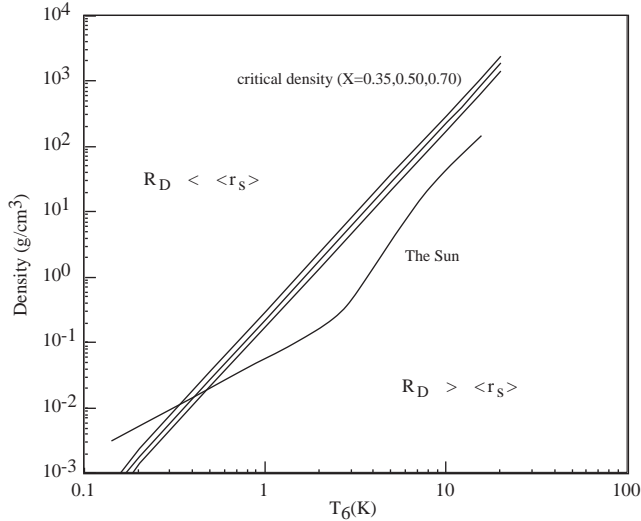
The relation of  $\langle r_z \rangle$  or  $\langle r_s \rangle$  to  $R_D$  is interesting. The condition  $\langle r_s \rangle = R_D$  can be written as

$$\rho_{crit} (\text{g cm}^{-3}) = 1.57(1 + 3X)^2 \left( \frac{T_6}{3 + X} \right)^3. \quad (13)$$

For densities below the critical density, the mean interparticle distance is smaller than the Debye radius. Hence, when analyzing the possibility that an ion carries a bound elec-



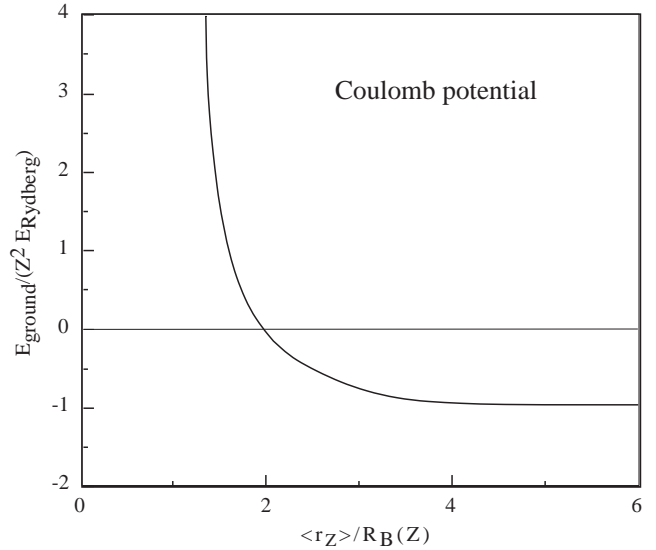
**Figure 5.** The run of the temperature ( $T_6$ ), the density, and the critical density as well as the Debye radius and the mean interparticle distance (the latter given in units of the Bohr radius for a  $Z = 4$  ion) in the Sun.



**Figure 6.** The temperature-density plane with the structure line of the Sun and the lines  $R_D = \langle r_s \rangle$  for three different values of the Hydrogen mass fraction, 0.35, 0.5 and 0.7. The almost straight part of the structure line is the convective zone.

tron, the Debye length is not relevant. In fig. 5 we show the run of the density and temperature in the Sun along with the critical density (calculated for the actual temperature and composition). Fig. 6 depicts the domains of  $R_D = \langle r_s \rangle$  for three values of the hydrogen mass fraction, 0.35, 0.5 and 0.7. One finds that through most of the volume of the Sun, the density is always below the critical one and hence the analysis of the structure of the electronic levels must take into account the nearby ion rather than the Debye radius. Only close to the surface does the situation change, the Debye radius becomes smaller than the mean interparticle distance and the critical density becomes smaller than the actual density.

When one evaluates the pressure ionization for metals at  $T = 0$ , one assumes the Wigner Seitz cell. The rational



**Figure 7.** The energy of the ground state of an ions with charge  $Z$  immersed in a plasma inside a unit cell of size  $\langle r_Z \rangle$ .

for using it at higher temperatures is the fact that the speed of the electron in the bound state is so much greater than the speed of the ions, such that the ions can be assumed to be at rest. The use of the ion-sphere for opacity calculations was examined by ?).

## 4.2 Schrödinger equation with Coulomb potential

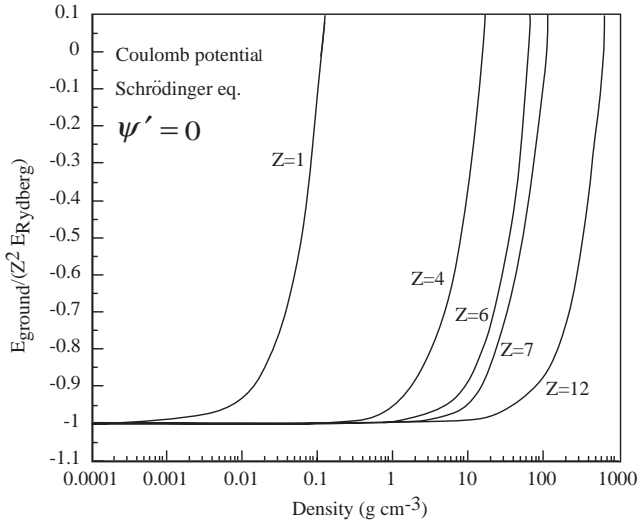
We used the variational principle method and trial functions of two types. The first type is taken from ?), namely a polynomial in  $r$  times an exponential function (the simple bound  $s$ -state), while the second type is a Padé approximation.

The results for Hydrogen obtained using the two types of trial functions are compared and found to be practically the same to within a relative accuracy of  $10^{-2}$  or better. Additional trials with other functions and parameters did not improve the results beyond the second significant digit.

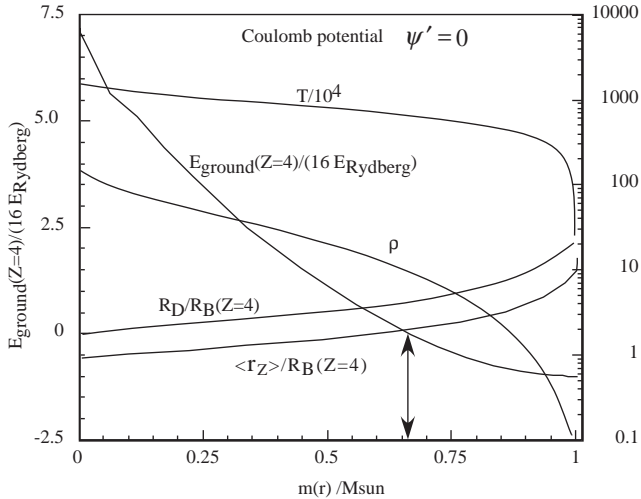
Interestingly, with our definition of  $\langle r_Z \rangle$ , the energy level is only a function of  $\langle r_Z \rangle / R_B(Z)$  and it is shown in fig. 7. Complete pressure ionization is found to occur at  $\langle r_Z \rangle = 1.945 R_B(Z)$  irrespective of  $Z$ . To obtain the results for a particular ion, one has to find its  $\langle r_Z \rangle$  for the composition, temperature and density under consideration. The results for  $T = 0$  are shown in fig. 8. We stress that these results are obtained for  $T = 0$  and do not depend on the Debye radius (and hence do not depend on the temperature indirectly). We conclude that neither  $\text{Ne}^{20}$ , nor species with a higher  $Z$ , are fully ionized in the solar core.

The above results are easily translated into the conditions in the Sun. In fig. 9, we plot the run of the ground state binding energy of  $\text{Be}^7$  throughout the Sun. This calculation indicates that Beryllium is fully ionized in the Sun below a solar mass fraction of 0.66.

The critical densities for the disappearance of the bound state in the corresponding Hydrogen like ions are given in Table 1. At a finite temperature, complete ionization takes places at somewhat lower densities because the temperature increases the excitation and with it the probability of ionization.



**Figure 8.** The translation of the previous figure to the density dependence of the energy levels of various species. All calculations assume that the  $Z \neq 1$  ions are trace elements.



**Figure 9.** The run of the ground level of  $\text{Be}^7$  in the Sun along with relevant thermodynamic parameters. On the left is the ground energy level axis. The axis for all other quantities is on the right. Temperature is given in  $10^4 \text{K}$ , density in  $\text{g cm}^{-3}$ . The arrow marks the point of complete ionization.

We conclude that the densities at which full ionization of  $\text{Be}^7$  takes place are significantly lower than those found in the solar core. Thus, the small inaccuracies in the present estimate have no practical effect on the state of Be in the solar core. The effect on the entropy density of the envelope is yet another issue, and it will be discussed elsewhere.

### 4.3 A Screened Potential?

The Schrödinger equation was solved using the simple Coulomb potential. It did not incorporate the Debye screened potential. However, electron screening does take place and cannot be ignored. Should the Debye screened potential be used? Suppose that  $R_D \gg \langle r_s \rangle$  (which is not the case in the Sun), namely there are many particles in the

Debye sphere. The Debye sphere contains electrons and ions, hence under these conditions there are ions which are closer to the specific ion than the Debye radius. These ions disturb the given ion and one should look for the bound level under these conditions, namely that there is another ion close by. This is exactly what has been done above. Thus, when the Debye radius is very large relative to the mean interparticle distance it creates a constant potential at the location where the two close particles are and the effect is a shift in the energy and pressure ionization of the very high energy levels. On the other hand, when  $R_D \approx \langle r_s \rangle$  the Debye length and potential lose their meaning. This is exactly the situation in the solar core. A full treatment of this limit which incorporate a Debye (or a more accurate) potential would have led to a still lower densities for the disappearance of the bound state).

### 4.4 The Kohn-Sham equation

There are two major deficiencies in the above treatment. The first one was discussed at length and has to do with the doubtful validity of the Debye potential under solar conditions and for the question of Be pressure ionization. A possible way to overcome this problem is to use a density functional (cf. ? where it is applied to Hydrogen plasma and where bound states are found). The second deficiency is the neglect of the free electrons and their effect on the screening of the nucleus, correlations and exchange. We therefore resorted to the Kohn-Sham equation (?), in which these deficiencies are taken care of, for finding the density at which pressure ionization takes place. The Kohn-Sham equation takes the  $N$  electron wave function and treats it as a collection of single particle eigenfunctions. The governing equation of the Kohn-Sham density functional method is then:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_l(\mathbf{r}) + \left[ -\frac{Ze}{\mathbf{r}} + e^2 \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} - \left( \frac{3}{\pi} n(\mathbf{r}) \right)^{1/3} \right] \psi_l(\mathbf{r}) = E_l \psi_l(\mathbf{r}). \quad (14)$$

where  $n(\mathbf{r})$  is the electron density and  $\psi_l$  is the single electron wave function. The Kohn-Sham equation (hereafter KS equation) has additional merits (?). The major problem with Thomas Fermi equation is that high densities do not necessarily lead to high kinetic energies for the electrons. This problem is cured in the above KS equation. There are more merits of using the KS equation in our particular problem. In the Hartree-Fock approach, the many-body wave function in form of a Slater determinant plays the key role in the theory. The Hartree-Fock equation if derived by minimization of the total energy is expressed by a determinant of wave functions which is extremely difficult to handle. In the density functional theory the key role is played by the observed quantity, the electron density. The Hohenberg-Kohn theorem then shows that for ground states the density functional theory possess an exact energy functional and there exists a variational principle for the electron density. The KS equation is then an effective one electron equation where the exchange operator in the Hartree-Fock equation is replaced by an exchange-correlation operator that depends only on the electron density. This is exactly what is needed in the



present problem. The KS equation then treats the  $N$  electron problem as single electron wave functions.

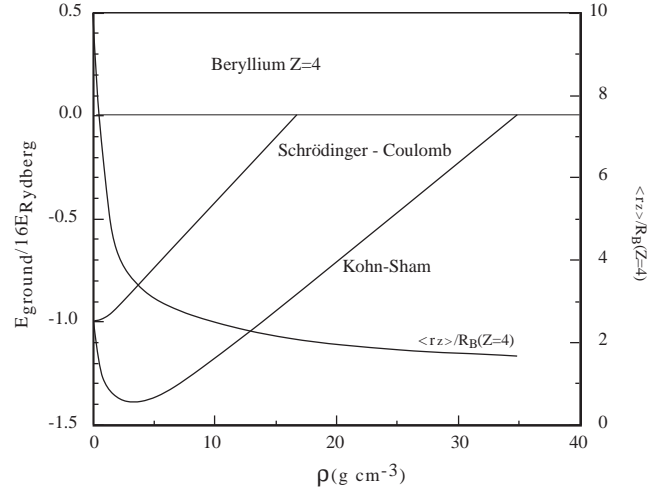
Let  $n(\mathbf{r}) = \sum_{l=1}^N |\psi_l(\mathbf{r})|^2$ , where the summation is carried over all electrons, be the electron density. In our particular case, we examine the bound state of Be ( $Z=4$ ) (as well as that of the higher  $Z$  trace species like C, N etc). The Be is a trace element immersed in a plasma of fully ionized Hydrogen and Helium (mostly) and negligible amounts of heavy elements. Hence, the major contribution to the electron density comes from the electrons contributed by Hydrogen and Helium. This term is essentially given by the environment in which the trace specie is immersed. Returning to the KS equation, the third term in the KS equation is the mutual electron-electron interaction between the bound electron and the free electrons which exist inside the ‘effective orbit’ and it provides the effective electron screening of the ion. It is easy to estimate when this term becomes important. The number of free electrons per Bohr radius,  $N_B$  is given by:

$$N_B \simeq \frac{6.16 \times 10^{-25}}{Z^3} n_e \quad (15)$$

This term becomes important for  $N_B \sim 1$  or  $n_e \gtrsim 1.623 \times 10^{24} Z^3$ . The forth term is the exchange which is given by  $\partial E_{ex}/\partial n$  where  $E_{ex}$  is the exchange energy. Because of its unique properties, the KS equation gained popularity with physical chemists. The accuracy of using the KS equation for the calculation of ionization potentials in molecules is described in (?). As a rule, the results of the KS equation are more accurate than those obtained from the Hartree-Fock approximation and reach the accuracy required by quantum chemists. The implementation of the KS equation in astrophysics of dense matter is described for the first time by (?).

We solved for the eigenvalue of the KS equation assuming the composition of the present solar core. We used a variational principle with several trial functions since we are mostly interested in the eigenvalues and not in the wave functions. The results for Be<sup>7</sup> are shown in figure 10 along with the results for the Coulomb potential (and the same boundary condition). It appears that the correlations and exchange terms in the KS equation contribute to the further suppression of the energy level and complete ionization occurs a la KS at a higher density. Note that for sufficiently low densities, the KS predicts significant lowering of the ground state of a *trace* element relative to the continuum. This is a consequence of the exchange term which is mostly contributed by Hydrogen and Helium and not by the electrons of the trace ion under consideration. The phenomenon does not occur for species which are not trace elements (see later). The results with different trial functions vary a bit and shown are the best (lowest) results. The critical densities and  $\langle r_Z \rangle$  as obtained in the two approximations are compared in Table 1. From the table we see that in the Schrödinger approximation  $\langle r_Z \rangle$  is constant while in the KS equation it varies and increases with the charge of the ion. A good fit for the value of the critical  $\langle r_Z \rangle$  over this range of charges is  $r_Z/Z = 0.451 - 0.026Z$ . This expression can be easily translated into a term added to the free energy so as to secure pressure ionization.

Based on the KS equation we find that the CNO elements are fully ionized in the core of the sun. Indeed, at



**Figure 10.** A comparison between the Muffin-Tin models employing the Schrödinger and the Kohn-Sham equations. Also shown is the radius of the atomic cell  $r_Z$  in units of the Bohr radius for a Hydrogen like ion with  $Z = 4$  treated as a trace element. The ground state energy level varies almost linearly with the density when close to the complete ionization density.

**Table 1.** The Critical Density and the radius of the atomic cell for the Vanishing of a Bound State in Hydrogen Like Ions

Ion Units	$\rho_{crit}(Coul)$ g cm <sup>-3</sup>	$\langle r_Z \rangle$ $R_B(Z)$	$\rho_{crit}(KS)$ g cm <sup>-3</sup>	$\langle r_Z \rangle$ $R_B(Z)$
Be <sup>7</sup>	16.33	1.921	36.18	1.474
C <sup>12</sup>	65.25	1.923	86.25	1.752
N <sup>14</sup>	110	1.922	132.5	1.806
O <sup>16</sup>	171	1.927	196.5	1.840
Mg <sup>24</sup>	660	1.925	698.8	1.890

$T = 0$  the Oxygen still has a bound electron at the densities of the solar core, but the low binding energy and the high temperature impose complete ionization under the conditions in the center of the Sun. On the other hand, species with  $Z \geq 10$ , like Neon and Iron, still keep their K-shell electrons. Assuming that all species heavier or equal to Ne are fully ionized introduces a relative error of the order of  $\lesssim Z(1 - X(C) - X(N) - X(O))/10$ , or about  $10^{-3}$  in the pressure and speed of sound.

#### 4.5 The effect of the boundary condition in the Kohn-Sham equation

The effect of the boundary condition on the result can be seen in the following way. We solved the KS equation under the condition  $\psi(r \rightarrow \infty) = 0$  for various densities. The result is that as the density increases monotonically, the first bound state becomes monotonically more bound and pressure ionization never occurs. The free electrons are able to prevent ionization exactly like the Saha equation with electron degeneracy, which yields that the free electrons recombine as the density increases.



#### 4.6 Metallic Beryllium

?) applied the Neutral-Pseudo Atom (NPA) method to evaluate the equation of state and the degree of ionization of pure Be metal under normal conditions ( $\rho = 1.85 \text{ g cm}^{-3}$  and  $T = 0$ ) and at high densities, keeping  $T = 0$ . The results are not directly applicable to the Sun because Perrot discusses pure metallic Beryllium while we are interested in a trace Be atom embedded in a sea of protons and  $\alpha$  particles. Yet, the results are instructive for the comparison of the present method with others, especially because they serve as a consistency check. The applicability of the NPA method (?) is limited to compression ratios  $c$  below 40 (see fig. 5 in the ? and the explanation therein) while Be becomes fully ionized at compression ratio of  $c = 50$ . At high compressions, band calculations show that the gap between the 1s band and the upper one close (?). The normal density of Beryllium is  $1.85 \text{ g cm}^{-3}$  and hence a compression ratio of 50 corresponds to a density of  $92.5 \text{ g cm}^{-3}$ . Consequently, Metallic Beryllium is fully pressure ionized at  $T = 0$  and a density of  $92.5 \text{ g cm}^{-3}$ . (?) presents an extrapolation between the end point of his results ( $c = 40$ ) and the band calculations ( $c = 50$ ).

We note that when the density or temperature (or both) are increased starting from  $\rho = 92.5 \text{ g cm}^{-3}$  and  $T = 0$  no bound state can re-appear. There is simply no bound state at higher densities and/or higher temperatures if it does not exist for  $T = 0$  and a given density.

Our calculations of the pressure ionization assume that the heavy elements under considerations are trace elements. Yet, it is of interest to compare the present method with others. The above results for metallic Beryllium provide such an opportunity. When the specie under consideration is a trace element, the electrons are contributed by the Hydrogen and Helium and there is no connection between the number of electrons in a unit cell and the charge of the ion. (There is no condition of charge neutrality per each ion sphere. The number of electrons in the Beryllium ion sphere is not necessarily 4). In the pure Beryllium case, when we search for the density of complete ionization, we assume that the free electrons are the first three electrons of Beryllium and that the forth one is bound. Thus the exchange term is evaluated on the basis of Beryllium ionized three times.

As can be deduced from the previous calculation, a critical factor is the packing of the specie. If spherical packing is assumed, then the KS equation predicts complete ionization at  $\rho \approx 56 \text{ g cm}^{-3}$ . On the other hand, (?) quotes that complete ionization is reached at  $92.5 \text{ g cm}^{-3}$ . The exact lattice structure of Beryllium at very high densities is not known and Be apparently undergoes a structural change at a compression ratio of about 3. However, if we assume an fcc lattice structure and resort to the appendix in (?) to find the relation between the lattice structure and the radius of the atomic cell ( $r_i = (\sqrt{2}/4)a$ ) we find complete ionization at a density of  $89.3 \text{ g cm}^{-3}$ , in good agreement with (?). This result reassures that our analysis for  $\text{Be}^7$  as a trace element is valid as well.

#### 5 THE EFFECT OF BE FULL IONIZATION ON THE SOLAR NEUTRINO FLUX

When Beryllium is completely pressure ionized in the core of the Sun, electron capture by Be takes place via the continuum only. Consequently, no corrections to the rate due to bound electrons should apply.

The effect of the complete ionization of  $\text{Be}^7$  on the solar neutrino flux can be easily estimated without recourse to detailed solar models because  $\text{Be}^7$  is a trace element and the amount of energy released by its reactions is negligible. Two facts are relevant. (a) The  $\text{Be}^7$  electron capture neutrino flux and the  $\text{B}^8$  flux are proportional to the abundance of  $\text{Be}^7$ . (b) The rate of electron capture is much larger than the rate of proton capture. Consequently, a decrease of about 20-30% in the rate of the  $\text{Be}^7 + e^-$  capture increases the abundance of  $\text{Be}^7$  by the same factor and hence increases the  $\text{B}^8$  neutrino flux by the same factor. The flux of the  $\text{Be}^7 + e^-$  neutrinos is unchanged because the decrease in the rate is fully compensated for by the increase in the abundance. As a matter of fact, the rate of  $\text{Be}^7 + e^-$  is determined (under the condition that the rate of  $\text{Be}^7 + e^-$  is much larger than the rate of  $\text{Be}^7 + p$ ) only by the rate of  $\text{He}^3 + \text{He}^4$ . The above treatment of the pressure ionization of  $\text{Be}^7$  applies to all solar models irrespective of any other parameter. The effect on the predicted flux assuming few different sets of nuclear parameters is shown in Table 2. The four models referred to in the table are the following. *Cas97* refers to (?), *DS96* refers to (?), *RMP98* refers to (?) and *NACRE* refers to (?). The models differ mainly in the parameters for the rates of the nuclear reaction and slightly in the details of the equation of state.

#### 6 CONCLUSION

In this work, we were interested in the internal structure of a trace ion in a high density plasma, and not in the general properties of the plasma. The relevant physical quantity for the latter, is the effective charge of an ion—not the electronic structure provided the effective radius of the electronic wave function is much smaller than the Debye radius. As to the structure of the ion itself, we distinguished between two cases depending on whether the mean interparticle distance is smaller or larger than the Debye radius. We found that throughout most of the Sun, the mean interparticle distance is slightly smaller than the Debye radius.

Under such conditions, the ionization state of a given ion depends mostly on the distance to the nearest neighbor rather than the distance scale of the screened potential. Hence, we approximate the condition of the plasma by a generalized Wigner-Seitz cell around each ion plus the proper boundary condition on the surface of the cell. We then impose the Bloch condition on the boundary of the generalized Wigner-Seitz cell. The fact that the nearest neighbor is so close implies that the implementation of this condition has a major effect on the point at which complete ionization takes place.

We have calculated the critical density of complete ionization assuming at first the Schrödinger equation and a Coulomb potential. Next, we implemented the Kohn-Sham equation which takes into account the exchange interaction

**Table 2.** The effect of treating the Be as fully ionized on the solar neutrino flux

	Cas97		DS96		RMP98		NACRE	
	full	partial	full	partial	full	partial	full	partial
$\phi(B^8)/10^6 \text{cm}^{-2} \text{s}^{-1}$	6.36	5.33	3.74	3.13	6.20	5.19	6.30	5.28
$\phi(B^8)10^3/\phi(Be^7)$	1.42	1.19	0.935	0.783	1.25	1.05	1.25	1.04
Ga(SNU)	133	133	121	121	132	132	137	137
Cl(SNU)	9.14	7.80	5.90	5.10	8.96	7.65	9.29	7.96

due to the free electrons and the screening by them. Comparison of our results with the NPA method yields a very good agreement for the case of metallic Beryllium.

We mention that when the boundary condition implemented in the KS equation is  $\psi(r \rightarrow \infty) = 0$  the phenomenon of pressure ionization disappears.

The improvements in the treatment of pressure ionization of trace elements show that all species with  $Z \leq 8$  are fully ionized in the core of the Sun. (The critical density for Oxygen is a bit higher than the density in the core of the Sun but the high temperature secure the complete ionization of Oxygen). The frequently applied correction to the  $\text{Be}^7$  electron capture rate due to bound electrons, is not needed. The revised prediction for the  $\phi_\nu(B^8)$  from the Sun is higher by about 20-30%.

The discussion here was centered around the high density effects. However, one should take into account collective effects as well (cf. ?). The energy of the electron plasma oscillations is

$$\hbar\omega_e = 3.7 \times 10^{-11} \sqrt{n_e} \text{ eV}. \quad (16)$$

At an electron number density of  $10^{26}$  the energy of the plasma oscillations amounts to 370 eV more than the ionization potential of  $\text{Be}^7$ . Thus the bound states of  $\text{Be}^7$  have been broadened into continuum states long before.

## 7 ACKNOWLEDGMENT

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